CLAIMS

What Is Claimed Is:

- 5
- 1. A bi-stable molecular mechanical device comprising a molecular system configured within an electric field generated by a pair of electrodes and electrically connected thereto, said molecular system having one rotor portion connected between two stator portions, wherein said rotor portion rotates with respect to said stator portions between at least two different states upon application of said electric field, thereby inducing a band gap change in said molecular system, wherein in a first state, there is extended conjugation over at least most of said molecular system, resulting in a relatively smaller band gap, and wherein in a second state, said extended conjugation is destroyed, resulting in a relatively larger band gap.
- 15

10

- 2. The molecular device of Claim 1 wherein said molecular system has an orientation axis and wherein said rotor portion is oriented perpendicular to said orientation axis, with said external electric field applied parallel to said orientation axis.
 - 3. The molecular device of Claim 2 wherein said molecular system comprises:

20

where

5

10

A is an Acceptor group comprising an electron-withdrawing group selected from the group consisting of: (a) hydrogen, (b) carboxylic acid and its derivatives, (c) sulfuric acid and its derivatives, (d) phosphoric acid and its derivatives, (e) nitro, (f) nitrile, (g) hetero atoms selected from the group consisting of N, O, S, P, F, Cl, and Br, (h) functional group with at least one of said hetero atoms, (i) saturated or unsaturated hydrocarbons, and (j) substituted hydrocarbons;

Less Conductive State (Off State)

D⁺ is a Donor group comprising an electron-donating group selected from the group consisting of: (a) hydrogen, (b) amines, (c) OH, (d) SH, (e) ethers, (f) saturated or unsaturated hydrocarbons, (h) substituted hydrocarbons, and (i) functional groups with at least one of hetero atom selected from the group consisting of B, Si, N, O, S, P, and I, wherein said Donor group is more electropositive than said Acceptor group;

Con₁ and Con₂ are connecting units between a molecule and a solid substrate selected from the group consisting of a metal electrode, an inorganic substrate, and an organic substrate, said connecting units independently selected from the group consisting of: (a) hydrogen (utilizing a hydrogen bond), (b) multivalent hetero atoms selected from the group consisting of C, N, O, S, and P, (c) functional groups containing said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (d) substituted hydrocarbons;

 G_1 , G_2 , G_3 , and G_4 are bridging groups for connecting said stator to each rotor or to connect two or more conjugated rings to achieve a desired electronic property, said bridging groups selected from the group consisting of: (a) hetero atoms selected from the group consisting of N, O, S, and P, (b) functional groups with at least one of said hetero atoms, (c) saturated or unsaturated hydrocarbons, (d) substituted hydrocarbons, (e) a single atom bridge, and (f) a direct sigma bond between said rotor and each stator; and

Q is a connecting unit between two phenyl rings and is selected from the group consisting of: (a) S, (b) O, (c) NH, (d) NR, (e) hydrocarbon, and (f) substituted hydrocarbon, and where the vertical dashed lines represent said solid substrate to which said molecule is electrically attached.

20

5

10

15

4. The molecular device of Claim 3 wherein said molecular system comprises:

where:

5

 R_1 and R_2 are independently hydrogen or hydrocarbon; and Y is selected from the group consisting of hydrogen, OH, and SH.

5. The molecular device of Claim 1 wherein said molecular system has an orientation axis and wherein said rotor portion is oriented parallel to said orientation axis, with said external electric field applied perpendicular to said orientation axis.

6. The molecular device of Claim 5 wherein said molecular system comprises:

On State (More Conductive State)

Switch On Switch Off
$$R_3 \xrightarrow{R_2} R_1$$

$$R_3 \xrightarrow{R_2} R_1$$

$$Con_1 \xrightarrow{G_1} G_2 \xrightarrow{G_3} G_3$$

$$R_1 \xrightarrow{G_2} R_2$$

$$R_2 \xrightarrow{R_2} R_3$$

$$R_1 \xrightarrow{R_2} R_3$$

$$R_1 \xrightarrow{R_2} R_3$$

Off State (Less Conductive State)

5 where:

A is an Acceptor group comprising an electron-withdrawing group selected from the group consisting of: (a) hydrogen, (b) carboxylic acid and its derivatives, (c) sulfuric acid and its derivatives, (d) phosphoric acid and its derivatives, (e) nitro, (f) nitrile, (g) hetero atoms selected from the group consisting of N, O, S, P, F, Cl, and Case 10003869

Br, (h) functional groups with at least one of said hetero atoms, (i) saturated or unsaturated hydrocarbons, and (j) substituted hydrocarbons;

D⁺ is a Donor group comprising an electron-donating group selected from the group consisting of: (a) hydrogen, (b) amines, (c) OH, (d) SH, (e) ethers, (f) saturated and unsaturated hydrocarbons, (g) substituted hydrocarbons, and (i) functional groups with at least one of hetero atom selected from the group consisting of B, Si, N, O, S, P, and I, wherein said Donor group is more electropositive than said Acceptor group;

5

10

15

20

25

30

Con₁ and Con₂ are connecting units between one molecule and another molecule or between a molecule and a solid substrate selected from the group consisting of a metal electrode, an inorganic substrate, and an organic substrate, said connecting units independently selected from the group consisting of: (a) hydrogen (utilizing a hydrogen bond), (b) multivalent hetero atoms selected from the group consisting of C, N, O, S, and P, (c) functional groups containing said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (e) substituted hydrocarbons;

R₁, R₂ and R₃ are spacing groups for providing an appropriate 3-dimensional scaffolding to allow molecules to pack together while providing rotational space for each rotor, said spacing groups selected from the group consisting of: (a) hydrogen, (b) saturated or unsaturated hydrocarbon, and (c) substituted hydrocarbon;

G₁, G₂, G₃, G₄, G₅, G₆, G₇, and G₈ are bridging groups for connecting said stator to each rotor or to connect two or more conjugated rings to achieve a desired electronic property, said bridging groups selected from the group consisting of: (a) hetero atoms selected from the group consisting of N, O, S, and P, (b) functional groups with at least one of said hetero atoms, (c) saturated or unsaturated hydrocarbons, (d) substituted hydrocarbons, (e) a single atom bridge, and (f) a direct sigma bond between said rotor and each stator; and

 J_1 and J_2 are tuning groups to provide at least one appropriate functional effect selected from the group consisting of inductive effects, resonance effects, and steric effects, said tuning groups being selected from the group consisting of: (a) hydrogen, (b) hetero atoms selected from the group consisting of N, O, S, P, B, F, Cl, Br and I, (c) functional groups with at least one of said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (e) substituted hydrocarbons;

7. The molecular device of Claim 6 wherein said molecular system comprises:

More Conductive State (On State)

Less Conductive State (Off State)

wherein the letters A, D, E, G, and J indicate sites where different chemical units can be utilized to adjust geometrical structure and optical properties of said molecular system and have generic designations as follows: A, D, E, G, and J are independently selected from the group consisting of heteroatoms, hydrocarbons (either saturated or unsaturated), and hydrocarbons with at least one said heteroatom, and where in addition to the foregoing, the letters G and J are independently selected from the group consisting of hydrogen, F, Cl, Br, and I.

10

15

20

5

- 8. The molecular device of Claim 1 comprising a crossed-wire device comprising a pair of crossed wires that form a junction where one wire crosses another at an angle other than zero degrees and at least one connector species connecting said pair of crossed wires in said junction, said junction having a functional dimension in nanometers, wherein said at least one connector species comprises said molecular system.
- 9. The molecular device of Claim 8 wherein said crossed-wire device is selected from the group consisting of memories, logic devices, multiplexers, demultiplexers, configurable interconnects for integrated circuits, field-programmable gate arrays (FGPAs), cross-bar switches, and communication devices.
- 10. The molecular device of Claim 1 wherein said molecular system is connected to said pair of electrodes by connector units.

25

11. A bi-stable molecular molecular system having one rotor portion connected between two stator portions, wherein said rotor portion rotates with respect to said stator portions between at least two different states upon application of said electric field, thereby inducing a band gap change in said molecular system, wherein in a first

30 state, there is substantial extended conjugation throughout said molecular system, re-

sulting in a relatively smaller band gap, and wherein in a second state, said extended conjugation is destroyed, resulting in a relatively larger band gap.

- 12. The molecular system of Claim 11 wherein said molecular system has an orientation axis and wherein said rotor portion is oriented perpendicular to said orientation axis, with said external electric field applied parallel to said orientation axis.
 - 13. The molecular system of Claim 12 comprising:

where

10.

5

A is an Acceptor group comprising an electron-withdrawing group selected from the group consisting of: (a) hydrogen, (b) carboxylic acid and its derivatives, (c) sulfuric acid and its derivatives, (d) phosphoric acid and its derivatives, (e) nitro, (f)

nitrile, (g) hetero atoms selected from the group consisting of N, O, S, P, F, Cl, and Br, (h) functional group with at least one of said hetero atoms, (i) saturated or unsaturated hydrocarbons, and (j) substituted hydrocarbons;

D⁺ is a Donor group comprising an electron-donating group selected from the group consisting of: (a) hydrogen, (b) amines, (c) OH, (d) SH, (e) ethers, (f) saturated or unsaturated hydrocarbons, (h) substituted hydrocarbons, and (i) functional groups with at least one of hetero atom selected from the group consisting of B, Si, N, O, S, P, and I, wherein said Donor group is more electropositive than said Acceptor group;

Con₁ and Con₂ are connecting units between a molecule and a solid substrate selected from the group consisting of a metal electrode, an inorganic substrate, and an organic substrate, said connecting units independently selected from the group consisting of: (a) hydrogen (utilizing a hydrogen bond), (b) multivalent hetero atoms selected from the group consisting of C, N, O, S, and P, (c) functional groups containing said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (d) substituted hydrocarbons;

G₁, G₂, G₃, and G₄ are bridging groups for connecting said stator to each rotor or to connect two or more conjugated rings to achieve a desired electronic property, said bridging groups selected from the group consisting of: (a) hetero atoms selected from the group consisting of N, O, S, and P, (b) functional groups with at least one of said hetero atoms, (c) saturated or unsaturated hydrocarbons, (d) substituted hydrocarbons, (e) a single atom bridge, and (f) a direct sigma bond between said rotor and each stator; and

Q is a connecting unit between two phenyl rings and is selected from the group consisting of: (a) S, (b) O, (c) NH, (d) NR, (e) hydrocarbon, and (f) substituted hydrocarbon, and

where the vertical dashed lines represent said solid substrate to which said molecule is electrically attached.

14. The molecular system of Claim 13 comprising:

25

5

10

15

20

where:

5

 R_1 and R_2 are independently hydrogen or hydrocarbon; and Y is selected from the group consisting of hydrogen, OH, and SH.

15. The molecular system of Claim 11 wherein said molecular system has an orientation axis and wherein said rotor portion is oriented parallel to said orientation axis, with said external electric field applied perpendicular to said orientation axis.

Less Conductive State (Off State)

16. The molecular system of Claim 15 comprising:

On State (More Conductive State)

Switch On Switch Off
$$R_3 \xrightarrow{R_2} R_1$$

$$Con_1 \xrightarrow{G_1} G_2 \xrightarrow{G_3} G_3$$

$$R_1 \xrightarrow{R_2} G_3$$

$$R_2 \xrightarrow{G_3} G_4$$

$$R_3 \xrightarrow{R_1} G_2$$

$$R_3 \xrightarrow{R_2} R_1$$

$$R_2 \xrightarrow{R_2} R_3$$

$$R_1 \xrightarrow{R_2} R_3$$

Off State (Less Conductive State)

5 where:

A is an Acceptor group comprising an electron-withdrawing group selected from the group consisting of: (a) hydrogen, (b) carboxylic acid and its derivatives, (c) sulfuric acid and its derivatives, (d) phosphoric acid and its derivatives, (e) nitro, (f) nitrile, (g) hetero atoms selected from the group consisting of N, O, S, P, F, Cl, and Case 10003869

Br, (h) functional groups with at least one of said hetero atoms, (i) saturated or unsaturated hydrocarbons, and (j) substituted hydrocarbons;

D⁺ is a Donor group comprising an electron-donating group selected from the group consisting of: (a) hydrogen, (b) amines, (c) OH, (d) SH, (e) ethers, (f) saturated and unsaturated hydrocarbons, (g) substituted hydrocarbons, and (i) functional groups with at least one of hetero atom selected from the group consisting of B, Si, N, O, S, P, and I, wherein said Donor group is more electropositive than said Acceptor group;

5

10

15

20

25

30

Con₁ and Con₂ are connecting units between one molecule and another molecule or between a molecule and a solid substrate selected from the group consisting of a metal electrode, an inorganic substrate, and an organic substrate, said connecting units independently selected from the group consisting of: (a) hydrogen (utilizing a hydrogen bond), (b) multivalent hetero atoms selected from the group consisting of C, N, O, S, and P, (c) functional groups containing said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (e) substituted hydrocarbons;

R₁, R₂ and R₃ are spacing groups for providing an appropriate 3-dimensional scaffolding to allow molecules to pack together while providing rotational space for each rotor, said spacing groups selected from the group consisting of: (a) hydrogen, (b) saturated or unsaturated hydrocarbon, and (c) substituted hydrocarbon;

G₁, G₂, G₃, G₄, G₅, G₆, G₇, and G₈ are bridging groups for connecting said stator to each rotor or to connect two or more conjugated rings to achieve a desired electronic property, said bridging groups selected from the group consisting of: (a) hetero atoms selected from the group consisting of N, O, S, and P, (b) functional groups with at least one of said hetero atoms, (c) saturated or unsaturated hydrocarbons, (d) substituted hydrocarbons, (e) a single atom bridge, and (f) a direct sigma bond between said rotor and each stator; and

 J_1 and J_2 are tuning groups to provide at least one appropriate functional effect selected from the group consisting of inductive effects, resonance effects, and steric effects, said tuning groups being selected from the group consisting of: (a) hydrogen, (b) hetero atoms selected from the group consisting of N, O, S, P, B, F, Cl, Br and I, (c) functional groups with at least one of said hetero atoms, (d) saturated or unsaturated hydrocarbons, and (e) substituted hydrocarbons;

17. The molecular system of Claim 16 comprising:

More Conductive State (On State)

Less Conductive State (Off State)

wherein the letters A, D, E, G, and J indicate sites where different chemical units can be utilized to adjust geometrical structure and optical properties of said molecular system and have generic designations as follows: A, D, E, G, and J are independently selected from the group consisting of heteroatoms, hydrocarbons (either saturated or unsaturated), and hydrocarbons with at least one said heteroatom, and where in addition to the foregoing, the letters G and J are independently selected from the group consisting of hydrogen, F, Cl, Br, and I.

10

5